

I. Improvements in the 2D TEP Neutral Particle Transport Calculation in Edge Plasmas (DoE Grant ER54538)

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Abstract

Extensions of the 2D Transmission and Escape Probability neutral particle transport method in treating the spatial non-uniformity of collision sources and neutral energy effects are presented. These extensions have been tested by benchmarks against Monte Carlo calculations for specially designed models and for realistic DIII-D discharges. The comparisons indicate these extensions improve accuracy of the TEP method.

1. Introduction

The Transmission and Escape Probability (TEP) method [1] and the 2D code GTNEUT [2] based thereon have been used to analyze 2D neutral particle transport for realistic edge models of plasma experiments. While comparisons of GTNEUT with Monte Carlo calculations of neutral measurements in DIII-D showed good agreement [3,4], extensive model problem testing identified certain limiting conditions for which some of the original TEP approximations could lead to inaccuracy [3,5]. We have previously described [6] an extension of the original DP0 approximation of the angular distribution of the incident neutral flux across interfaces to DP1 and DP2 to improve the accuracy of the calculation of transmission probabilities for models in which transmission across a series of optically thin regions would produce increasingly forward peaked anisotropic fluxes incident across successive interfaces. In this paper we report improved approximations which allow a more accurate treatment of 1) the preferential escape of scattered or charge-exchanged neutrals back across the incident surface in optically thick regions 2) the energy distribution of neutrals in optically thin regions in locations with strong background plasma ion temperature gradients.

2. Two Major Improvements

2.1 Correction to escape probabilities

The TEP method is based on the particle current balance [1] across each interface between any two contiguous computational regions. An exiting current from a region is coupled to all incoming currents from all the adjacent regions via transmission and escape probabilities.

$$\Gamma_{i,j}^n = \sum_{k,n'} T_{i,k \rightarrow j}^{n' \rightarrow n} \Gamma_{k,i}^{n'} + \sum_{k,n'} \left(\delta_{n'0} - \sum_l T_{i,k \rightarrow l}^{n' \rightarrow 0} \right) \Gamma_{k,i}^{n'} c_i P_i \Lambda_{ij}^0 \delta_{n0} + S_{ext}^i P_i \Lambda_{ij}^0 \delta_{n0} \quad (1)$$

where $\Gamma_{i,j}^n$ is the n -th moment of the total partial current from region i to region j , $T_{i,k \rightarrow j}^{n' \rightarrow n}$ represent the transmission probability that neutral particles flowing from region k in moment n' to region i will be directly transmitted to region j in moment n without a collision within region i , P_i is the total escape probability that charge-exchanged and recombination neutrals or their progenies within region i escape into region j , $\Lambda_{i,j}^0$ is the directional escape probabilities that neutrals escaping from region i escape into region j , c_i is the charge exchange fraction and S_{ext}^i represents recombination neutral source rate.

The accuracy of the TEP method depends completely on transmission and escape probabilities. The DP₁ or DP₂ approximation of the angular distribution allows a more accurate evaluation of transmission probabilities for optically thin regions, but the calculation of collision probabilities was previously based on the flat collision source approximation. In this approximation, the collision source is assumed to be uniformly distributed over each computational region, implying that the collision source has no preferable escaping direction. Since the actual collision source is strongly peaked near the incident surface for an optically thick region, and consequently charge-exchanged neutrals are more likely to escape back across the incident surface than in any other directions. As a result, the flat collision source approximation leads to an over-predication of collided fluxes in the forward direction in optically thick regions.

The variational diffusion approximation used in this research to correct directional escape probabilities consists of three steps. First, the original problem with non-uniform first-collision sources resulting from

neutrals entering from all adjacent regions is separated into several simpler problems, within each of which we only deal with the first-collision source associated with neutrals entering from one of the contiguous regions. The linear separation in this step converts the original problem into collision response calculations, and therefore directionalities could be calculated if even the exact collision source distribution of the original problem is unknown. In the second step, the diffusion approximation (2) is used to describe neutral transport in an optically thick region.

$$-\nabla \cdot D \nabla \phi(r) + \Sigma_a \phi(r) = S_{j,i}^0(\mathbf{r}) \quad (2)$$

where $\phi(\mathbf{r})$ is the neutral scalar flux, D is the diffusion coefficient, Σ_{ion} is the total macroscopic ionizing cross section, $S_{j,i}^0(\mathbf{r})$ represents the first-collision source distribution associated with a flux entering from region j to region i . In the last step, each optically thick region is divided into a number of sub-regions (elements), finite element methods are applied to the diffusion equation (2) to obtain a piecewise linear flux representation, and finally the total and directional escape probabilities can be calculated.

In addition to the non-uniformity of the first collision rate within optically regions, angular fluxes along interfaces between regions are also characterized by a strong gradient, which couples the spatial non-uniformity of both uncollided and collided fluxes with contiguous regions. To take this effect into account, a spatially linear function is added to the set of original DP₁ representation functions [6].

$$\psi_{i,j}^3(x_{ij}, \mathbf{\Omega}) = \frac{2\sqrt{3}}{\pi L_{ij}^2} (x_{ij} - 0.5L_{ij}) \quad (3)$$

where L_{ij} is the length of the interface between regions i and j , $\psi_{i,j}^3(x_{ij}, \mathbf{\Omega})$ represents a spatially linear and angularly isotropic representation function. Here spatially linear DP₁ (and also linearly anisotropic) representation functions are not taken into consideration because they can always be regarded as higher order approximations either for optically thick or thin regions. Apparently, for optically thin regions, all the spatially linear terms can be neglected, while for optically thick region, it has been shown that all DP1 terms can be safely ignored because of the randomization of charge-exchanged scattering events.

The non-uniformity of uncollided fluxes is embodied in calculations of transmission probabilities, while the non-uniformity of collided fluxes is taken into account in diffusion calculations of escape probabilities. To the lowest order the following two linear contributions for the collided flux crossing an interface of a given region must be considered: (1) the spatially linear outgoing collided flux associated with a spatially uniform flux entering into that region, where the non-uniformity is driven by material attenuation; (2) the spatially linear collided angular flux associated with a spatially linear flux entering into that region, where the non-uniformity is driven by the non-uniform incoming flux and material attenuation.

2.2 Neutral energy treatment

The treatment of the neutral energy distribution has an important impact on accuracy of the TEP method. Transmission and escape probabilities are functions of the neutral mean free path (mfp), which depends on neutral energies. As a result, errors in the neutral energy treatment can propagate to the neutral partial current crossing each interface. The original TEP method used the local ion temperature (LIT) approximation, which basically assumed all neutrals from a region are in thermal equilibrium with ions in that region, resulting an average energy equal to the local ion temperature, i.e. $\bar{E} = T_i$, where T_i is the local ion temperature in region i . Extensive comparisons with Monte Carlo show that this is a good approximation when the mfp is small compared to the characteristic dimension of computational regions, or the local ion temperature changes slowly from region to region. However, for a long mfp region, neutrals from this region predominantly consist of uncollided neutrals directly transmitted from the adjacent regions, and if, at the same time, the local ion temperature changes dramatically across from region to region, the energy of collided neutrons are significantly different from the local ion temperature, and therefore the original approximation that the local neutral distribution could be represented as a Maxwellian with the local ion temperature becomes inadequate.

To remedy this defect, the average neutral energy (ANE) approximation used in this research calculates the average energy of neutrals flowing out across an interface as a weighted average of energies

of uncollided neutrals directly transmitted from all the contiguous regions and energies of charge-exchanged neutrals in the thermal equilibrium with the local ions within that region, i.e.

$$\bar{E}_{ij} = \frac{\sum_{k,n} T_{i,k \rightarrow j}^{n \rightarrow 0} \Gamma_{k,i}^n \bar{E}_{ki} + \Gamma_{i,j}^{c,0} T_i}{\sum_{k,n} T_{i,k \rightarrow j}^{n \rightarrow 0} \Gamma_{k,i}^n + \Gamma_{i,j}^{c,0}} \quad (4)$$

where \bar{E}_{ij} is the average energy of neutrals from region i to region j , $\sum_n T_{i,k \rightarrow j}^{n \rightarrow 0} \Gamma_{k,i}^n$ represents the uncollided current from region k to region j , $\Gamma_{i,j}^{c,0}$ is the collided current from region i to region j .

Before using Equation (4) to evaluate the average neutral energy, uncollided and collided currents across each interface must be known; to calculate these currents, we have first to compute transmission and escape probabilities, which implicitly depends on the neutral energy distribution. The neutral current balance equation must be solved iteratively. The iterative process is started with the local ion temperature approximation ($\bar{E}_{ij} = T_i$), and then the mfp, transmission and escape probabilities can be evaluated. After that, we can solve the linear equations (1) to obtain collided and uncollided fluxes, which can then be used to update the average neutral energy in Equation (4). Once the average neutral energies are well converged, neutral densities and reaction rates can be computed.

3. Results and discussion

In order to investigate the impact of the variation diffusion approximation on the accuracy of the TEP method, a test problem with a uniform background plasma is chosen to avoid errors introduced by neutral energy approximations. Similarly, vacuum boundaries are assumed on the four external interfaces, so that errors produced by the reflection models can be precluded. The problem shown in Fig. 1 consists of nine identical squares. A uniform neutral source with unit strength is imposed on the left boundary of region 2.

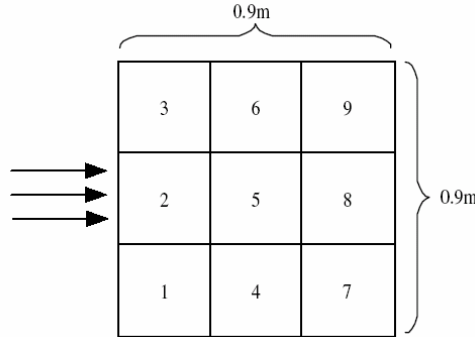


Fig.1 Geometry for the 2D nine-region configuration

Both the electron and ion temperatures are 10 eV. The charge exchange fraction and Δ/λ ratio are adjusted to be 0.9 and 5, respectively, resulting in a very strongly non-uniform collision source distribution of incident neutrals in region 2. Neutral densities calculated by DEGAS and GTNEUT with various approximations are shown in Fig. 2. It can be seen that GTNEUT with the DP_0 approximation significantly over-estimates neutral densities for regions away from the source, and there is no obvious improvement using the DP_1 approximation, since both calculations ignore the strong gradient of collision sources and angular fluxes in region 2. With the non-uniformity of collision sources taken into account, the diffusion approximation significantly improves agreement with the Monte Carlo calculations, but it still over-predicts the results for regions 4-9, since the effects of non-uniform flux along interfaces between regions are neglected. If both the diffusion and spatially linear angular flux approximation are used, the GTNEUT calculations are in excellent agreement with the DEGAS simulations.

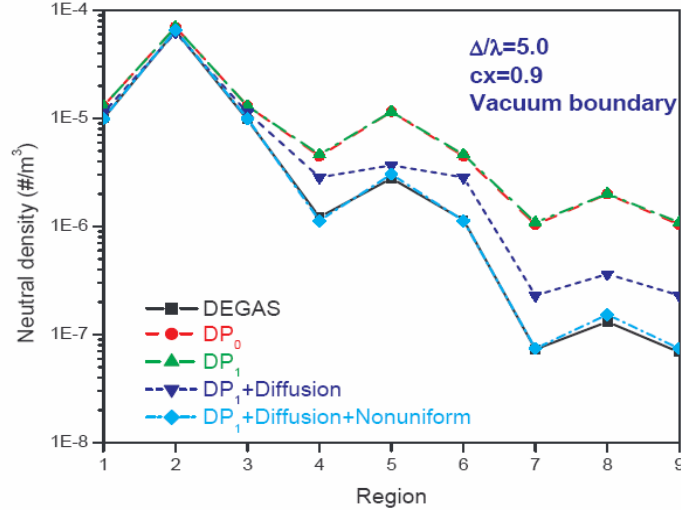


Fig.2 Neutral densities calculated by DEGAS and GTNEUT for the 2D model problem

In addition to specially designed model problems, realistic DIII-D discharges are also used to test the performance of the new extensions. The geometric configuration of the DIII-D discharge 96747 at 3940 ms is shown in Fig. 3, where the shaded regions represent the locations where neutral densities were measured. The problem is characterized by a strong gradient in the background plasma properties. For instance, the ion temperature varies from 57 eV in the private flux region to more than 600 eV inside the separatrix near the X-point. As a result, the neutral mean free path could be lower than 6 cm in the main plasma region, while it could be as high as 26 m outside the separatrix. Recycling neutral sources are imposed on bottom boundaries of regions 2-13, and for all regions, the grid size is much smaller compared to the mfp, resulting in three important effects on neutral transport in this specific problem: 1) strong anisotropy of angular fluxes, 2) almost uniform collision sources within each computational region, and 3) a big difference between energies of collided and uncollided fluxes.

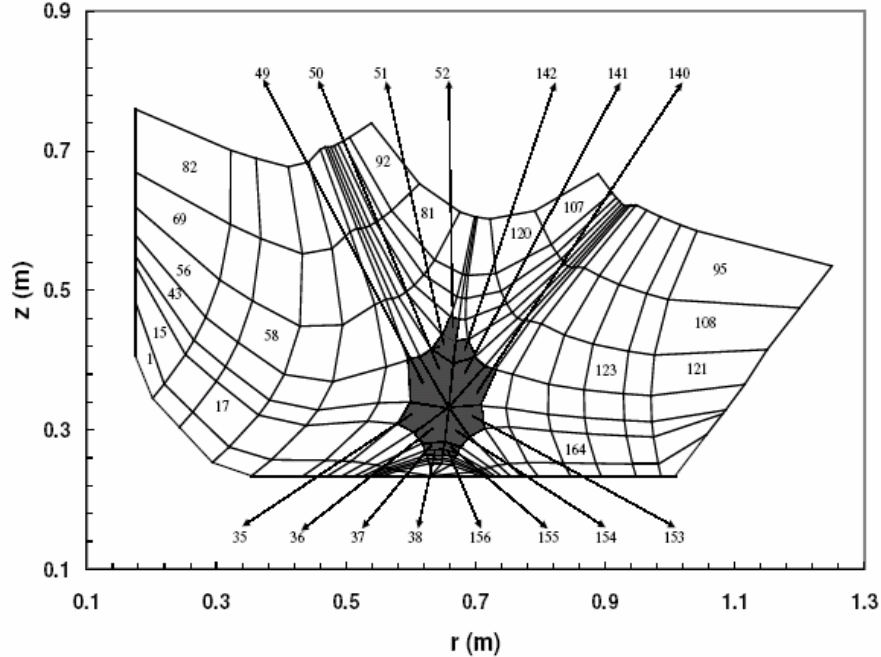


Fig.3 Geometry for the DIII-D H discharge 96747 at 3940 ms

The comparison of density calculations by DEGAS and GTNEUT with different level approximations is illustrated in Fig. 4. It can be seen that the ANE approximation is superior to the LIT approximation, since the energy of uncollided neutrals originating from carbon walls is much lower than that of collided neutrals, and consequently the LIT approximation cannot sufficiently represent the neutral energy distribution. The DP_1 approximation also improves agreement with DEGAS simulations, since in

optically thin regions neutral fluxes become strongly anisotropic. The diffusion approximation has no obvious improvement as we expected for large mean free path regions.

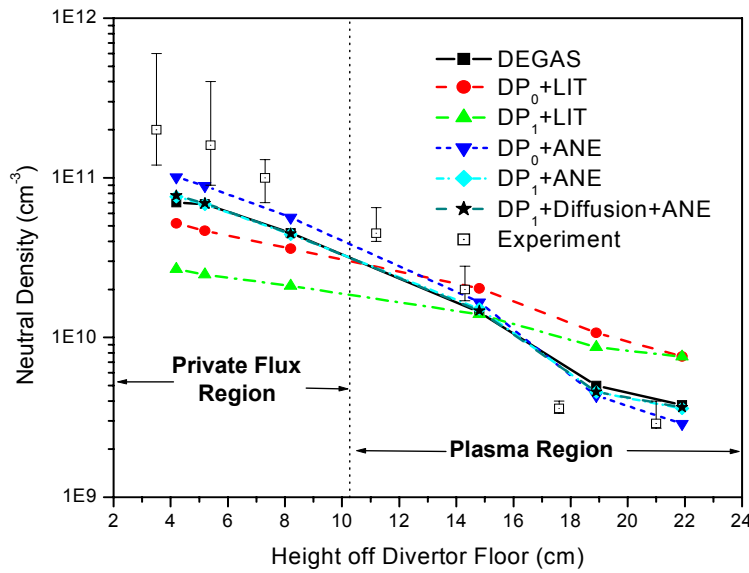


Fig.4 Neutral densities calculated by DEGAS and GTNEUT for the DIII-D H discharge

4. Conclusions

The variational diffusion and ANE approximations have been developed to extend the TEP method. Benchmark comparisons with Monte Carlo for model problems in which the mean free path was small relative to the dimension of the computational region indicate that the intra-nodal diffusion treatment of the escape probability directionality significantly improves accuracy in optically thick regions. Iterative calculation of average neutral energy in a region as the weighted average of the energies of neutrals incident from the contiguous regions and the energy of neutrals resulting from charge-exchanged ions within the region, has been found to yield improved and quite good agreement with continuous energy Monte Carlo calculations for both model problems and realistic DIII-D discharges.

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